Thin nanocrystalline films of silicon carbide (SiC) have been deposited on Si substrates by rf magnetron sputtering in pure Ar atmosphere. Simultaneously classical molecular dynamics (MD) simulations of sputtering of β-SiC by Ar atoms were performed using IMD and Materials Explorer software with a combination of the Tersoff and the Ziegler-Biersack-Littmark (ZBL) potential in order to get more insight into the sputter process. In experiments the bias voltage (0 to −40 V) has been varied at constant substrate temperature of 900 °C to investigate the influence on the composition, the constitution and the mechanical properties of crystalline β-SiC films. At second the substrate temperature has been varied between 900 °C and 100 °C to find the minimum substrate temperature that is needed to get nanocrystalline β-SiC under the applied sputter conditions (ceramic SiC target, 300 W rf power, 18 cm target-substrate distance, 50 sccm Ar gas flow, 0.26 Pa total gas pressure). The films have been characterized by electron probe micro-analysis (EPMA), X-ray diffraction (XRD), Raman spectroscopy and atomic force microscopy (AFM). Hardness and residual stress have been investigated by nanoindentation and wafer bending. In the MD simulations the sputter yield was determined as a function of the energy of the incident Ar atoms (in the interesting range for sputter deposition, i.e., 50–1000 eV). To our knowledge this is the first time that the sputter yield of a SiC target was determined as a function of the energy of the incident Ar atoms in the low energy range by using MD simulations and compared with experimental results.

Keywords: Magnetron Sputtering, Silicon Carbide, Nanoindentation, Molecular Dynamics Simulation, Sputter Yield.

1. INTRODUCTION

Due to their mainly covalent bonding silicon carbide (SiC) thin films are of great scientific and technological interest because of their excellent properties such as good corrosion and wear resistance, high hardness, chemical inertness, high thermal stability and good electric conductivity. These material characteristics make it attractive for semiconductor applications (high temperature electronics, high frequency devices, optoelectronic application), for protective coatings against corrosion of steel, X-ray mask materials and protection of thermonuclear reactor walls. SiC can appear in different crystal structures: in a metastable, cubic low temperature modification (β-SiC) and in various rhombohedral or hexagonal high temperature modifications (α-SiC), which form from β-SiC above 1000 °C. The polytypes of α-SiC differ in the orientation and the stacking sequence of subsequent tetrahedron layers. The most common types are 4-H-, 6-H- und 15-R-α-SiC. A great advantage of SiC is that the mechanical properties of the α- and the β-phase do not differ as much as in the case of graphite/diamond or cubic and hexagonal boron nitride. Moreover under high compressive stress β-SiC can become superhard.

Various techniques have been applied to deposit crystalline SiC films such as: CVD,1–8 reactive and non-reactive magnetron sputtering,9–14 molecular ion beam deposition,15,16 pulsed laser deposition17,18 and ion implantation.19 For industrial applications crystalline SiC coatings are mainly deposited by chemical vapour deposition (CVD)
Sputter Deposition of Nanocrystalline β-SiC Films and MD Simulations of the Sputter Process

Ziebert et al.

at typical deposition temperatures of more than 1000 °C. These CVD methods usually use hydrogen-containing process gases such as methane (CH\textsubscript{4}), silane (SiH\textsubscript{4}) or HMDS (Si(CH\textsubscript{3})\textsubscript{4}), which can lead to a high content of bonded hydrogen (10–30 at.%) in the growing films, and thus to SiC\textsubscript{x}H\textsubscript{y} coatings. To deposit hydrogen-free SiC coatings, the PVD methods are more appropriate, because they can also work with pure Ar process gas. Generally, at low deposition temperatures (T < 700 °C) and medium or high growth rates (R ≥ 5 nm/min) sputtered SiC coatings are amorphous. However, Ulrich et al.\textsuperscript{10} succeeded in depositing hard nanocrystalline β-SiC coatings with a crystallite size of 20 nm by r.f. magnetron sputtering of a SiC target in pure argon plasma at a low substrate temperature of only 420 °C. They showed that intense argon ion bombardment (high ion flux and low ion energies) during film growth and low growth rates (R < 5 nm/min) are required.

In the case of large systems (number of atoms > 1000) the classical molecular dynamics (MD) method is well suited for the simulation of structural and mechanical properties of materials at the atomic scale. In this method the atoms of a solid are regarded as point particles, which interact by classical potential functions. The Newton equations of motion are numerically integrated, with the possibility to take into account certain conditions, such as external forces or deformations and to use various thermodynamic ensembles, such as the canonical NVT ensemble (i.e., a system with a constant volume in contact with a heat bath of constant temperature). From the configurations, which are calculated in the MD simulation, energies, stresses, distortions and elastic constants can be locally determined. For the simulation of covalent solids, as in the case of SiC/Si\textsubscript{3}N\textsubscript{4} multilayer films, multi-body potentials are necessary, because directed bonds are occurring. These potentials can be subdivided into two main categories, on the one hand those potentials, which can be split into two- and three-body parts and on the other hand, the bond-order potentials. The most popular potential of the first class is the Stillinger-Weber potential,\textsuperscript{20} for the second class the most popular representative is the Tersoff potential.\textsuperscript{21, 22}

Sputtering is the removal of target atoms by ion bombardment. The quantitative value for this removal is the sputtering yield, defined as the number of removed atoms or molecules per incident ion. To simulate the sputter process in the thin film deposition the ZBL (Ziegler-Biersack-Littmark) potential was developed\textsuperscript{23} and later combined with the multi-body potentials mentioned above. MD simulations of sputter processes make especially sense for low process energies below 1 keV. At higher energies the single collision cascades are spatially separated and the binary collision approximation in the form of Monte Carlo (MC) simulations can be used,\textsuperscript{24} which is implemented in such widespread codes as TRIM\textsuperscript{25} and TRIDYN.\textsuperscript{26} In 1988 Harrison made pioneering work when he investigated collision cascades by MD simulations using the simple pair potentials for metals and noble gases available at that time. He showed important principles, such as e.g., channelling and blocking mechanisms of surface atoms, which are responsible for the emission pattern of the sputtered particles.\textsuperscript{27} For the bombardment of covalent materials similar sputter mechanisms were found, but the open lattice structures allowed stronger contributions from the second and third atomic layers as in the case of metals.\textsuperscript{28} In 2002 Ecke et al. compared the experimental sputter yields of SiC for bombardment of Ar ions in the energy range between 0.5 and 5 keV under 60° sputtering with MC simulations using the programs TRIM and T-DYN. They reported that the differences between the results of the simulation programs are sometimes greater than their difference from the experimentally measured sputter yields.\textsuperscript{29} Later Kosiba performed TRIDYN simulations and compared them to his experimental results from Auger spectroscopy.\textsuperscript{30} In 2004 Shapiro et al. investigated the influence of the interatomic potential on the results of MD simulations of the sputter process and showed that most sputter parameters are relatively independent on the choice of the potential.\textsuperscript{31}

Our overall research goal is to use molecular dynamics simulations in combination with experimental validation for the development of improved SiC and Si\textsubscript{3}N\textsubscript{4} single- and bilayer coatings, and multilayer SiC/Si\textsubscript{3}N\textsubscript{4} nanolaminates, which are deposited by magnetron sputtering onto silicon and/or steel. As the first experimental step thin SiC films have been deposited by rf magnetron sputtering with systematic variation of the substrate temperature and the bias voltage and the influence of these deposition parameters on the constitution, the microstructure and the mechanical properties were investigated to find out, whether it is possible to deposit nanocrystalline b-SiC films with the chosen sputter set-up. As the first MD simulation step the sputtering of a β-SiC-target at 700 K by argon was simulated using the Tersoff potential for the Si–C interaction and tabulated ZBL pair potential for the interaction with argon. Of course it would have been nice to compare the experimental results of a deposition process directly with MD simulations. However, for the MD simulations it is necessary at first to get more insight into the sputtering process, because this gives the necessary input parameters for the MD simulation of the SiC deposition process. To our knowledge this is the first time that the sputter yield of a SiC target was determined as a function of the energy of the incident Ar atoms in the low energy range by using MD simulations and compared with experimental results.

2. EXPERIMENTAL DETAILS

2.1. Deposition

The SiC-films were produced in a PVD-CVD hybrid coating machine consisting of an electron cyclotron
resonance (ECR) microwave plasma beam source, an ECR-microwave ion gun, three magnetron sputter sources (target-substrate distance 18 cm) and a heatable substrate holder where a variable substrate bias voltage can be applied. The films were prepared in unbalanced rf magnetron sputtering mode at a power of 300 W at substrate temperatures between 100 and 900 °C and bias voltages up to −40 V without making use of the ECR components. The target was a hot pressed SiC target (diameter = 75 mm, thickness = 6 mm, purity = 99.95%). Double-side polished, (100)-oriented silicon wafers were used as the substrates. Prior to the film deposition, the substrates were ultrasonically cleaned in isopropanol, and additionally cleaned by argon ion beam etching for 10 min each at deposition temperature with a bias voltage of −400 V. The base pressure before deposition was lower than 3 × 10⁻⁴ Pa and a working pressure of 0.26 Pa was adjusted by 50 sccm Ar gas flow.

2.2. Characterization

The coating thickness has been measured by a surface profilometer (type Tencor P-10). Chemical composition was investigated by using EPMA (type Cameca Camebax Microbeam). The surface topography was studied by means of AFM (Digital Instruments Inc., Dimension 3100) with a Si tip (Nanosensors LFM-20; tip radius < 10 nm) in contact mode. The crystal structure was investigated by XRD (Seifert Company, PAD II) with Cu Kα radiation. The measured diffractograms have been fitted by pseudo-Voigt functions using the Rietveld program LS1 developed by Lutterotti et al., which allows the determination of the crystallite sizes and the lattice constants. The bonding characteristics have been investigated by Raman spectroscopy (type Renishaw micro-Raman spectroscopy system 1000). As mechanical properties, nanohardness H, reduced Young’s modulus E’ (CSIRO, UMIS2000) and residual stress σr (wafer bending method, type Tencor P-10) were measured. Nanohardness and reduced Young’s modulus were determined from load versus penetration depth curves using the Oliver-Pharr method and the ASMEC Indentanalyser software at a maximum applied load of 10 mN to reduce both the influence of the surface roughness and of the substrate.

3. COMPUTATIONAL METHODS

By classical molecular dynamics the sputter process for the β-SiC target material by Ar atoms was simulated to get additional information on the expected sputter yields. For the modelling of the short-range interaction, the tabulated ZBL potential was used and for modelling the Si–C interaction the Tersoff classical potential was chosen, which has been used before successfully in several SiC studies. Especially when the overall computational workload is massive, using the Tersoff potential is better than tight-binding or ab initio potentials. For the MD simulations both the commercial software package Materials Explorer 4.0 (ME) (Fujitsu Ltd.) and the MD program package IMD (ITAP Molecular Dynamics), which was developed at the university of Stuttgart and is suited for many platforms from a single PC to a massively parallel supercomputer, were used. A comparison of these two different software packages seems interesting, because they have different advantages and disadvantages which have to be compared and if possible their advantages combined to get better MD simulation results. E.g., ME possesses a better graphical interface and is easier to use, but the maximum block size is limited. In both cases periodic boundary conditions were applied at the lateral (x, y) boundaries to mimic a semi-infinite surface and remove edge-effects and the simulations cells had an open top layer in the +z direction. In the ME simulations, i.e., those performed with the ME software, the C-terminated β-SiC single crystal target has a size of 8 × 8 × 12 units cells consisting of 6144 atoms with the density of about 3.3 g/cm³. In the IMD simulations the dimensions are 10 × 10 × 20 unit cells, i.e., 16000 atoms. The chosen unit cell size for the ME is the maximum size that can be simulated by the Materials Explorer Software, which is running on a single Windows workstation. Because the IMD software, which is running in parallel on a high performance cluster, allows a larger unit cell size, this larger size was chosen for the IMD simulations. The chosen cell height made sure that the incident Ar ions transfer all their energy to the SiC target and the chosen cell width ensures that the Ar ions do not hit the boundaries.

The same number of Si and C atoms was initially placed on the diamond lattice and an equilibration of the target at 673 K for 1 ps using the NPT-ensemble with external pressure control by the Parinello-Rahman method and temperature control by the Nose-Hoover thermostat which was developed at the University of Stuttgart and is suited for many platforms from a single PC to a massively parallel supercomputer. After the equilibration the atoms in the two bottom layers were fixed to prevent unphysical centre-of-mass drift of the lattice caused by the momentum transfer from the bombarding ion.

To simulate the sputter process two different procedures were applied using the microcanonical NVE ensemble. In the ME simulations an area of 1.2 nm × 1.2 nm was chosen on the SiC (001) surface. Starting at a height of 2 nm above the surface one randomly oriented (on the x–y plane) Ar ion at an incident angle of 0°, measured from the macroscopic surface normal, with a fixed energy of 1 eV was allowed to impact this surface area. For the IMD simulations 9 coordinates were defined according to the crystal...
Sputter Deposition of Nanocrystalline $\beta$-SiC Films and MD Simulations of the Sputter Process

Ziebert et al.

Fig. 1. Definition of the 9 coordinates for a C-terminated SiC-surface.

The symmetry of the zincblende structure as shown schematically in Figure 1, and for every coordinate the MD simulations were performed for one Ar ion that impacts the SiC (001) surface at this coordinate at 0° and fixed energy. Coordinate Nr. 1 is an atom of the topmost C layer, coordinate Nr. 2 is an atom of the layer below, which is the first Si layer, Nr. 3 is in the third layer, i.e., the second C layer and Nr. 4 is in the second Si layer. The other coordinates are selected in the centres between the layers (Nr. 5–8) and in the free space (Nr. 9). Thus there is no covalent Si–C bonding for Nr. 5 in contrast to Nr. 6, 7 and 8, which are situated below by $1/4$ of the lattice constant.

The experimental sputtering yield is an average of numerous sputtering events. In simulations, especially at higher energies, the yield can vary from zero to several thousand atoms per ion between individual events. A single large yield event can increase the average yield significantly and the results are very sensitive to whether a single event is included in an average or not. To compare simulated results to experimental values it is necessary to run enough simulations with different random initial values. Therefore in both procedures 50 simulations have been performed for every ion energy in order to stabilize the calculated average sputter yield. A simulation time of 2 ps was chosen to ensure that the individual atoms oscillate around a momentarily stable average distance from their equilibrium bulk positions after the impact. The sputter yield was calculated from the final states of the simulations as a function of the incident energy of the argon ions, which was varied between 50 eV and 1 keV, which is the interesting range for sputter deposition. An atom or an atom cluster is considered sputtered, if it is more than 0.6 nm away from the surface, which is twice the cut-off distance of the potentials. Furthermore, the trajectories of the Ar atoms and the ranges of Ar ions and sputtered Si and C atoms were determined from the simulation data.

4. RESULTS AND DISCUSSION

4.1. Experimental Results

4.1.1. Constitution

4.1.1.1. Thickness and Composition. At a deposition time of 9 h the thickness of all films was between 1.8 and 2.2 $\mu$m. The lower curves in Figure 2 show the argon, oxygen, nitrogen, silicon, and carbon atomic concentrations of the SiC films deposited without bias voltage as a function of the substrate temperature, as measured by EMPA. The argon and the oxygen concentration are constantly below 0.7 at.% and 1.1 at.% respectively, whereas the nitrogen concentration shows a small increase from around 2 at.% up to a maximum of 3.7 at.% at 700 °C. The reason for this nitrogen contamination is not yet clear. Possible explanations could be that is due to the SiC target itself or due to a Si$_3$N$_4$ target which was already in the chamber during deposition because in further experiments the deposition conditions for SiC/Si$_3$N$_4$ multilayers should be studied. Up to 600 °C the concentrations of silicon and carbon remain almost constant at about 43 at.% and 53 at.%. With increasing substrate temperature the Si concentration shows a small decrease to 40.5 at.%, while the C concentration increases to 55.5 at.%. Thus the SiC$_x$ films have an increasing x value of 1.23–1.37, or a decreasing Si/C ratio of 0.82–0.73 (Fig. 2, upper curve), which means an increasing C excess of about 19–27%. To bring more light into the nature of this carbon phase content Raman spectra at a laser wavelength of 514.5 nm have been recorded that reveal that the films contain carbon in amorphous form as an addition to the $\beta$-SiC phase, because the typical D and G bands for a-C have been found. The evaluation of the
Raman spectra showed that with increasing substrate temperature the D and G bands show an increasing separation, which indicates increasing graphitisation. This graphitisation is even more pronounced for the film with higher substrate bias. Concerning the dependence of the chemical composition on the bias voltage at constant substrate temperature of 900 °C no significant dependence was found. In contrast to Lattemann et al.\textsuperscript{14} no decreasing Si concentration due to increasing resputtering of Si was observed with increasing bias voltage.

4.1.1.2. Crystal Structure. Figure 3 shows the evolution of the X-ray diffractograms for films deposited with increasing substrate temperature from 600 °C to 900 °C without bias voltage in the 2θ-range from 25 to 50°. Up to 600 °C the SiC films are amorphous. At 700 °C a broad peak appears at around $2\theta = 35.6°$ which can be assigned to the (111) peak of the $\beta$-SiC phase. With increasing substrate temperature this peak narrows and increases in intensity, indicating an increase in crystallinity and crystallite size. No other peaks can be detected, especially no peaks of the $\alpha$-SiC phase which leads to the conclusion that a nanocrystalline strongly (111)-textured $\beta$-SiC film has been deposited. To answer the question, whether the film is textured or epitaxial, transmission electron microscopy has to be performed in future work, which will also help to find out, whether the a-C found in the Raman spectra is textured or epitaxial, transmission electron microscopy has to be performed in future work, which will also help to find out, whether the a-C found in the Raman spectra forms a grain boundary or a matrix phase. For 700 °C the crystallite size determined from Rietveld refinement is 17 nm, it increases to 32 nm at 800 °C and finally to 41 nm at 900 °C. Concerning the determined lattice parameters of 0.435–0.4375 nm, they are in reasonable agreement with the literature value $a = 0.4358$ nm (JCPDS card #75-0254). A similar crystallite size of 20 nm was found by Liao et al.\textsuperscript{16} for pure nanocrystalline $\beta$-SiC films deposited by thermal plasma chemical vapour deposition on molybdenum substrates at a much higher substrate temperature of 1250 °C.\textsuperscript{46} A low bias voltage of $U_s = -10$ V leads to a further increase in crystallinity and crystallite size to 49 nm. At higher values of the bias voltage the crystallite size decreases again and reaches 23 nm at $U_s = -40$ V. The related lattice constant shows an increase from 0.4365 nm to 0.44 nm with increasing bias voltage indicating an increase in residual stress, which also affects the adhesion and the mechanical properties.

4.1.1.3. Surface Topography. In Figure 4(a) comparison between the AFM surface topography images (scan size 1 $\mu$m $\times$ 1 $\mu$m) of SiC films deposited at 600 °C (Fig. 3(a)), 700 °C (Fig. 3(b)) and 900 °C (Fig. 3(c)) is shown. At 600 °C only diffuse features with a maximum height below 1 nm can be seen, which confirms the amorphous nature of this film. The image of the film deposited at 700 °C shows small rounded structures with an average diameter of 7 nm as determined by the grain size analysis method of the Nanoscope AFM software. This size which can be regarded as the lateral crystallite size of the nanocrystalline films increases to 9 nm for a substrate temperature of 900 °C. From the AFM topography images the average roughness values $R_s$ and the vertical distance from the deepest valley to the highest peak values $R_h$ have been determined using the average of five images taken at a scan size of 10 $\mu$m $\times$ 10 $\mu$m. Up to a substrate temperature of 600 °C the films are amorphous, the surface is very smooth and the values for $R_s$ and $R_h$ are below 0.4 nm and 8.4 nm respectively. At 700 °C both roughness parameters show a large increase to 9 nm and 88 nm, indicating the onset of recrystallization. With further increasing substrate temperature they decrease again to 4 nm and 55 nm.

4.1.2. Mechanical Properties

The maximum penetration depth in the nanoindentation tests for the SiC films was 160 nm, which is less than 10% of the total film thickness of 2 $\mu$m. Thus the rule of thumb to minimize the substrate influence is fulfilled. The quotient of the residual depth and the maximum depth is smaller than 0.7 for all measurements independent of the deposition temperature with values ranging from 0.3 to 0.5. According to Bolshakov and Pharr this indicates that the pile-up effect can be neglected.\textsuperscript{47} Thus there is no indication that the elastic-plastic behaviour changes towards more plastic with the substrate temperature, which would lead to an overestimation of the hardness as determined by nanoindentation. Hardness $H$ and the reduced Young’s modulus $E^*$ of the SiC films are plotted in Figure 5(a) as a function of the substrate temperature. Both $H$ and $E$ show a similar increase with increasing substrate temperature starting at 23 GPa and 214 GPa respectively and a maximum in the hardness of 33 GPa and in the reduced Young’s modulus of 336 GPa is reached at a substrate temperature of 900 °C. These values are approximately equal to the value of standard bulk SiC. When the bias voltage is increased at this substrate temperature to $-10$ V the hardness and the reduced Young’s modulus increase up to 36 GPa and 348 GPa respectively. These values are...
Sputter Deposition of Nanocrystalline \( \beta \)-SiC Films and MD Simulations of the Sputter Process

Fig. 4. Comparison of the AFM surface topography images of SiC-films deposited at \( T_s = 600 \) °C (a), 700 °C (b), and 900 °C (c).

Fig. 5. Hardness and reduced Young’s modulus of the SiC films in dependence of: (a) The substrate temperature at \( U_s = 0 \) V. (b) The bias voltage at \( T_s = 900 \) °C.

less than the values of 45–55 GPa reported by Kulikovsky et al. for sputtered amorphous hydrogen-free a-C:Si films with about 40 at.% Si and comparable to the values of Liao et al. for crystalline hydrogenated SiC films deposited by CVD. A further increase in the bias voltage deteriorates the mechanical properties. Without applied bias voltage the residual stresses are compressive and remain at low levels below \(-0.7\) GPa up to 900 °C substrate temperature. The hardness increase with increasing substrate temperature seems therefore to be correlated with the increase in crystallite size (Fig. 3). The further increase in the hardness at \(-10\) V bias voltage can be attributed to an increase of the compressive stress to \(-2.2\) GPa. With further increasing bias voltage the stress level reaches high values of \(-12\) GPa at \(-30\) V and \(-20\) GPa at \(-40\) V leading to increasing adhesion problems.

4.2. Simulation Results

In Figure 6 the energy dependence of the sputter yields calculated with the IMD software for the 9 coordinates for a \( \beta \)-SiC crystal is shown for the energy range from 50 eV to 1 keV. The first singular sputtering events during the 50 IMD simulations are observed at argon impact energy of 50 eV at coordinate Nr. 6, when the argon ions hit the Si atoms of the second layer. For the ME simulations the sputter threshold energy is estimated to be
around 40 eV, which is in good agreement with the theoretical value of 41 eV of Kosiba. Kosiba determined the threshold from a fit of their TRIDYN data by the revised Bohdansky formula. At 90 eV the sputtering probability in the IMD simulations increases and at coordinate Nr. 6 a sputtering event occurs in more then 10% of the simulations. The sputter yield for this coordinate also shows the largest increase up to 1.6 molecules/ion, whereas the sputter yields for the coordinates Nr. 1–4 and Nr. 9 remain below 0.2 molecules/ion even at an incident energy of 1 keV. The other coordinates Nr. 5, 7 and 8 give maximal sputter yields in the range between 0.4 and 0.8 molecules/ion. Coordinates Nr. 1–4 are almost central collisions between the bombarding Ar ion and the Si and C atoms of the four top layers. Thus, if an Ar ion hits coordinates Nr. 1–4 it transfers all of his energy and impulse (in − z direction) to the target atom, which it transfers to the atoms situated below. Thus the entropy or randomness of the impulses is created some layers deeper in the target, which decreases the probability for a sputter event. This makes the formation of a collision cascade more difficult, which is necessary to give the target atom a direction towards the surface to finally get sputtered, i.e., leave the target material. On the contrast if the Ar ion hits coordinate Nr. 6, 7 or 8 it breaks a covalent bonding and because this represents a lateral collision, the energy in the upper layers is transferred in the x−y-plane, which leads to a higher sputter probability after some collision cascades. Thus the high sputter rate of the coordinate No. 6 is due to the fact that the uppermost C-atom has two open dangling bonds and if one of his remaining bonds is broken by a hitting Ar ion, it becomes very mobile and can transfer a lot of his energy to the neighbor atoms, which also are surface atoms that can be sputtered more easily. The coordinate Nr. 9 is chosen in the free space between the layers, which largely reduces the probability to hit a target atom. This leads to a low sputter yield. The red curve in Figure 6 represents the sputter yield averaged over the 9 coordinates. It reaches about 0.4 molecules/ion at 1 keV.

The averaged sputter yield from the IMD simulations for the energy range from 50 eV to 1 keV is compared in Figure 7 with the results from the ME simulations, with TRIM and TRIDYN MC simulations and with values for the experimental sputter yield taken from the literature. Experimental values for the low energy dependence of the sputtering yield for SiC by Ar ions are rarely published. Mostly there are experimental results for light projectiles like H, D, and He because of its importance in the nuclear fusion technology. Because in literature no experimental data have been found for the sputtering of a SiC (001) surface, the values for the sputter yield of SiC (0001) determined from target weight losses measured by an in-situ microbalance, by measuring the step height of mesa structures with a microinterferometer and by Auger depth profiling were chosen for comparison. However, Petzold et al. did not observe a dependence of the measured sputter yield on the polytype of the substrate.

Up to 600 eV there is a good qualitative and quantitative agreement between the ME values and the data from Comas and Cooper. Unfortunately they did not measure at higher energies. There is only one value of 0.46 molecules/ion at 1 keV from Petzold available and TRIM and TRIDYN calculations, which are in the same range. The experimental and TRIM values of Ecke et al. at 500 eV are a bit below those of Comas and of the ME simulations. However it has to be kept in mind, that the yields of Ecke have been determined for 60° incidence angle. Therefore in order to compare results obtained for 60° incidence angle with those for 0°, the results for 60° bombardment should be divided by the factor $\cos^2 \theta$ with $f$ as a fitting factor. Sigmund proposed the factor $f$ to be 5/3. Using this factor the experimental and the TRIM data points for 0° incidence, shown in Figure 7, have been calculated. Thus, there is some uncertainty due to a possible unknown variation of this factor with energy. The averaged IMD data for the sputter yield show good agreement up to
300 eV, but for higher energy they become too low. This indicates that it is too simple to use an unweighted average of the 9 coordinates for the comparison with experimental data. It will be necessary to account for a different probability for the collisions on the 9 coordinates to occur. However, in general, the agreement of experimental data with calculated values is reasonable, although there do exist some deviations.

5. SUMMARY AND CONCLUSIONS

As the first experimental step thin SiC films have been deposited by rf magnetron sputtering with systematic variation of the substrate temperature and the bias voltage and the influence of these deposition parameters on the constitution, the microstructure and the mechanical properties was investigated. At a small substrate bias voltage \(U_s = -10\) V and a substrate temperature \(T_s = 900^\circ\)C a nanocrystalline film with pure \(\beta\)-SiC phase was deposited. This film showed a high hardness of \(H = 36\) GPa at a reasonable compressive stress level of \(-2.2\) GPa. So it can be concluded that the rf magnetron sputtering is a suitable method to prepare hard nanocrystalline pure \(\beta\)-phase hydrogen-free SiC-films.

As the first molecular dynamics simulation step the sputtering of a \(\beta\)-SiC-target at 700 K by argon was simulated using the Tersoff potential for the Si–C interaction and tabulated ZBL pair potential for the interaction with argon. To our knowledge this is the first time that the sputter yield of a SiC target was determined as a function of the energy of the incident Ar atoms in the low energy range by using MD simulations and compared with experimental results. In general, the agreement of experimental data with values calculated by the two different molecular dynamics approaches is reasonable, although some deviations do exist, especially at higher energies. So it can be concluded that MD simulations are an effective approach to study the energy dependence of the sputter yield in order to find the energy for the maximum sputter yield and the threshold energy for the sputtering process.

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References and Notes


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